3,4-Difluorobenzyl alcohol, tert.-butyl ether

Inchi: InChI=1S/C11H14F2O/c1-11(2,3)14-7-8-4-5-9(12)10(13)6-8/h4-6H,7H2,1-3H3
InchiKey: XAHGLAMYUOPINE-UHFFFAOYSA-N
Formula: C11H14F2O
SMILES: CC(C)(C)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
gf	-356.89	kJ/mol	Joback Method
hf	-589.97	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	43.16	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.280		Crippen Method
mcvol	151.500	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1203.00		NIST Webbook
rinpol	1203.00		NIST Webbook
tb	505.45	K	Joback Method
tc	700.19	K	Joback Method
tf	291.02	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.02	J/mol×K	505.45	Joback Method
cpg	360.58	J/mol×K	537.91	Joback Method
cpg	374.36	J/mol×K	570.36	Joback Method
cpg	387.39	J/mol×K	602.82	Joback Method
cpg	399.71	J/mol×K	635.27	Joback Method
cpg	411.33	J/mol×K	667.73	Joback Method
cpg	422.29	J/mol×K	700.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume